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Essential self–adjointness of symmetric linear relations associated to first order systems

Matthias Lesch

Abstract

The purpose of this note is to present several criteria for essential self–adjointness. The method is based on ideas due to Shubin.

This note is divided into two parts. The first part deals with symmetric first order systems on the line in the most general setting. Such a symmetric first order system of differential equations gives rise naturally to a symmetric linear relation in a Hilbert space. In this case even regularity is nontrivial. We will announce a regularity result and discuss criteria for essential self–adjointness of such systems. A byproduct of the regularity result is a short proof of a result due to Kogan and Rofe–Beketov [8]: the so–called formal deficiency indices of a symmetric first order system are locally constant on $\mathbb{C} \setminus \mathbb{R}$. The regularity and its corollary are based on joint work with Mark Malamud. Details will be published elsewhere.

In the second part we consider a complete Riemannian manifold, M, and a first order differential operator, $D : C_0^\infty(E) \to C_0^\infty(F)$, acting between sections of the hermitian vector bundles E, F. Moreover, let $V : C^\infty(E) \to L^\infty_{\mathrm{loc}}(E)$ be a self–adjoint zero order differential operator. We give a sufficient condition for the Schrödinger operator $H = D^t D + V$ to be essentially self–adjoint. This generalizes recent work of I. Oleinik [11, 12, 13], M. Shubin [16, 17], and M. Braverman [2].

We essentially use the method of Shubin. Our presentation shows that there is a close link between Shubin's self–adjointness condition for the Schrödinger operator and Chernoff's self–adjointness condition for powers of first order operators.

We also discuss non–elliptic operators. However, in this case we need an additional assumption. We conjecture that the additional assumption turns out to be obsolete in general.

The criteria we are going to present in the first and second part of this note are very closely related. In fact, after we had done the second part, we saw that the theory can be extended to symmetric linear relations associated to symmetric first order systems.

Contents

1. First order systems on the line

Let $I \subset \mathbb{R}$ be an interval. We consider a first order system

$$J(x)\frac{df}{dx} + B(x)f(x) = \mathscr{H}(x)g(x), \tag{1.1}$$

where

$$\begin{aligned}
&J \in \mathrm{AC}(I, \mathrm{M}(n,\mathbb{C})), &&J(x) = -J(x)^*, \quad \det J(x) \neq 0, \text{ for } x \in I,\\
&B \in L^1_{\mathrm{loc}}(I, \mathrm{M}(n,\mathbb{C})), &&B(x) = B(x)^* - J'(x), \text{ for } x \in I, \\
&\mathscr{H} \in L^1_{\mathrm{loc}}(I, \mathrm{M}(n,\mathbb{C})), &&\mathscr{H}(x) = \mathscr{H}(x)^*, \quad \mathscr{H}(x) \geq 0, \text{ for } x \in I.
\end{aligned} \tag{1.2}$$

Here, $\mathrm{M}(n,\mathbb{C})$ denotes the set of complex $n \times n$ matrices and $\mathrm{AC}(I, \mathrm{M}(n,\mathbb{C}))$ the set of absolute continuous functions with values in $\mathrm{M}(n,\mathbb{C})$.

We need some more notation: we equip $C_0(I, \mathbb{C}^n)$, the space of continuous $\mathbb{C}^n$–valued functions with compact support, with the (semidefinite) scalar product

$$\langle f, g \rangle_{\mathscr{H}} := \int_I f(x)^* \mathscr{H}(x) g(x) dx, \tag{1.3}$$

and denote by $\mathscr{L}^2_{\mathscr{H}}(I)$ the completion of $C_0(I, \mathbb{C}^n)$ with respect to the semi-norm induced by (1.3). Alternatively, $\mathscr{L}^2_{\mathscr{H}}(I)$ can be described as the set of Borel–measurable $\mathbb{C}^n$–valued functions satisfying $\langle f, f \rangle_{\mathscr{H}} := \int_I f(x)^* \mathscr{H}(x) f(x) dx < \infty$. As usual, one puts $L^2_{\mathscr{H}}(I) := \mathscr{L}^2_{\mathscr{H}}(I)/\{f \in \mathscr{L}^2_{\mathscr{H}}(I) \mid \|f\|_{\mathscr{H}} = 0\}$. $L^2_{\mathscr{H}}(I)$ is a Hilbert space. For a function $f \in \mathscr{L}^2_{\mathscr{H}}(I)$ we will denote by $\widetilde{f}$ the corresponding class in $L^2_{\mathscr{H}}(I)$. If $\mathscr{H}(x)$ is invertible a.e. then a class $\widetilde{f}$ contains at most one continuous representative, hence if $\mathscr{H}(x)$ is invertible a.e. and f is continuous we will not distinguish between f and $\widetilde{f}$.

Assume for the moment that $\mathscr{H}(x)$ is invertible for almost all $x \in I$ and $\mathscr{H}(x)^{-1} \in L^1_{\mathrm{loc}}(I, \mathrm{M}(n,\mathbb{C}))$. Then (1.1) induces a symmetric operator

$$L := \mathscr{H}^{-1}\Big(J\frac{d}{dx} + B\Big) \tag{1.4}$$

in the Hilbert space $L^2_{\mathscr{H}}(I)$ with domain $\mathscr{D}(L) = \mathrm{AC}_{\mathrm{comp}}(I, \mathbb{C}^n)$. The symmetry is implied by $B = B^* - J'$ and $\mathscr{H}^* = \mathscr{H}$. However, the interesting case is the one where $\mathscr{H}(x)$ is singular. If $\mathscr{H}(x)$ is singular then (1.1) will in general neither define an operator nor will it be densely defined. Rather it will give rise to a *symmetric linear relation*, whose definition we recall for the reader's convenience:

Definition 1.1. Let $\mathfrak{H}$ be a linear space equipped with a positive semidefinite hermitian sesqui–linear form $\langle \cdot, \cdot \rangle$. A linear subspace $\mathscr{S} \subset \mathfrak{H} \times \mathfrak{H}$ is called a symmetric linear relation (s.l.r.) if for $\{f_j, g_j\} \in \mathscr{S}, j = 1, 2$, one has $\langle f_1, g_2 \rangle = \langle f_2, g_1 \rangle$.

For example, the graph of an (unbounded) symmetric operator in $\mathfrak{H}$ is a s.l.r. The system (1.1) defines a symmetric linear relation, $\mathscr{S}_{\min}$, in $\mathscr{L}^2_{\mathscr{H}}(I)$ as follows: $\{f, g\} \in \mathscr{S}_{\min}$ if and only if $f \in \mathrm{AC}_{\mathrm{comp}}(I, \mathbb{C}^n), g \in \mathscr{L}^2_{\mathscr{H}, \mathrm{comp}}(I)$ and $Jf' + Bf = \mathscr{H}g$.
$\mathscr{S}_{\min}$ induces a symmetric linear relation, $S_{\min}$, in $L^2_{\mathscr{H}}(I)$ in a fairly straightforward way: $\{\widetilde{f}, \widetilde{g}\} \in S_{\min}$ if and only if there exist representatives $f \in \widetilde{f}, g \in \widetilde{g}$ such that $\{f, g\} \in \mathscr{S}_{\min}$.
Looking at first order systems seems to be rather special. Therefore, it is important to note that an arbitrary symmetric n^{th}–order system is unitarily equivalent to a symmetric first order system ([8], [14]). In most cases, however, the Hamiltonian $\mathscr{H}$ of this first order system will be singular. As an example we show how a second order Sturm–Liouville equation can be transformed into a system of the form (1.1):

Example 1.2. We consider a Sturm–Liouville type equation

$$-\frac{d}{dx}\left(A(x)^{-1}\frac{d}{dx}u(x)\right) + V(x)u(x) = \mathscr{H}(x)v(x), \tag{1.5}$$

where $A, V, \mathscr{H} \in L^1_{\mathrm{loc}}(I, \mathrm{M}(n, \mathbb{C}))$ and $A(x)$ is positive definite for all $x \in I$. The system (1.5) defines a symmetric linear relation as follows: $\{u, v\} \in \mathscr{S}_{\min}$ if and only if $u \in \mathrm{AC}_{\mathrm{comp}}(I, \mathbb{C}^n), A^{-1}\frac{d}{dx}u \in \mathrm{AC}_{\mathrm{comp}}(I, \mathbb{C}^n), v \in \mathscr{L}^2_{\mathscr{H}, \mathrm{comp}}(I)$ and (1.5) holds. As before, let $S_{\min} := \{\{\widetilde{u}, \widetilde{v}\} \mid \{u, v\} \in \mathscr{S}_{\min}\}$.
Note that if $v \in \mathscr{L}^2_{\mathscr{H}, \mathrm{comp}}(I)$ then, since $\mathscr{H} \in L^1_{\mathrm{loc}}(I, \mathrm{M}(n, \mathbb{C})), \mathscr{H}v \in L^1_{\mathrm{comp}}(I, \mathbb{C}^n)$. Consequently, $\{(u, iA^{-1}\frac{d}{dx}u), (v, 0)\}$ is in the symmetric linear relation, $\widetilde{\mathscr{S}_{\min}}$, induced by the system

$$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}\begin{pmatrix} f_1 \\ f_2 \end{pmatrix}' + \begin{pmatrix} V & 0 \\ 0 & -A \end{pmatrix}\begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = \begin{pmatrix} \mathscr{H} & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} g_1 \\ g_2 \end{pmatrix}. \tag{1.6}$$

Conversely, if $\{(f_1, f_2), (g_1, g_2)\} \in \widetilde{\mathscr{S}_{\min}}$ then $\{f_1, g_1\} \in \mathscr{S}_{\min}$. It is also clear that the Hilbert spaces $L^2_{\mathscr{H}}(I)$ and $L^2_{\widetilde{\mathscr{H}}}(I), \widetilde{\mathscr{H}} = \begin{pmatrix} \mathscr{H} & 0 \\ 0 & 0 \end{pmatrix}$, are canonically isomorphic. Hence the s.l.r. $S_{\min}$ and $\widetilde{S}_{\min}$ in $L^2_{\mathscr{H}}(I)$ resp. $L^2_{\widetilde{\mathscr{H}}}(I)$ are unitarily equivalent.
If $\mathscr{H}(x)$ is invertible and $\mathscr{H}(x)^{-1} \in L^1_{\mathrm{loc}}(I, \mathrm{M}(n, \mathbb{C}))$ then $S_{\min}$ is (the graph of) a densely defined symmetric operator in the Hilbert space $L^2_{\mathscr{H}}(I)$. However, $\widetilde{\mathscr{H}}(x)$ is singular everywhere.

The following example shows that the domain of the s.l.r. $S_{\min}$ can be rather small:

Example 1.3. Let $B = 0, J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, and $\mathscr{H}(x) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$. If $\{f, g\} \in \mathscr{S}_{\min}$ then $f'_2 = g_1, f'_1 = 0$, and since f is absolute continuous with compact support we infer $f_1 = 0$. Hence $\mathscr{H}f = 0$ and thus $\widetilde{f} = 0$. Thus, the domain of $S_{\min}$ is $\{0\}$.

The system (1.1) can be simplified further and put into canonical form. Details of the construction can be found in [8, Sec. 1.3] or [10]. For the moment denote by $\mathscr{S}(J, B, \mathscr{H})$ the s.l.r. induced by the system (1.1). A "gauge transformation" $U \in \mathrm{AC}(I, \mathrm{GL}(n, \mathbb{C}))$ induces a unitary map

$$\Psi_U : \mathscr{L}^2_{\mathscr{H}}(I) \to \mathscr{L}_{\widetilde{\mathscr{H}}}(I), \quad f \mapsto U^{-1}f, \quad \widetilde{\mathscr{H}} := U^*\mathscr{H}U, \tag{1.7}$$

and a simple computation shows that

$$\Psi_U \mathscr{S}(J, B, \mathscr{H})\Psi_U^* = \mathscr{S}(\widetilde{J}, \widetilde{B}, \widetilde{\mathscr{H}}), \tag{1.8}$$

where

$$\widetilde{J} = U^*JU, \quad \widetilde{B} = U^*JU' + U^*BU, \quad \widetilde{\mathscr{H}} = U^*\mathscr{H}U. \tag{1.9}$$

It can be shown that the gauge transformation U can be chosen in such a way that J is constant and $B = 0$. Such a system is called "canonical".

Pick $x_0 \in I$ and let $Y(., \lambda) : I \to \mathrm{M}(n, \mathbb{C})$ be the solution of the initial value problem

$$J(x)Y'(x, \lambda) + B(x)Y(x, \lambda) = \lambda\mathscr{H}(x)Y(x, \lambda), \quad Y(x_0, \lambda) = I_n. \tag{1.10}$$

Here, I_n denotes the $n \times n$ unit matrix. The existence of Y follows from the integrability assumptions in (1.2).

Definition 1.4. The system (1.1) is said to be *definite* on I if there exists a compact subinterval $I_0 \subset I$ such that the matrix

$$\int_{I_0} Y(x, \lambda)^*\mathscr{H}(x)Y(x, \lambda)dx \tag{1.11}$$

is invertible for a $\lambda \in \mathbb{C}$.

If the system is definite then (1.11) is invertible for all $\lambda \in \mathbb{C}$ [8, Theorem 1.1]. The property of a system (1.1) to be definite is gauge invariant. There is a simple criterion for definiteness: namely, if there exists a compact subinterval $I_0 \subset I$ such that $\int_{I_0} \mathscr{H}$ is invertible, then the system is definite. For a canonical system ($B = 0$) this criterion is also necessary. In general, the definiteness will also depend on J and B.

Some bibliographic comments are in order, however we do not claim to give a complete historical account: A standard reference for symmetric linear relations arising from symmetric first order systems is the thesis of Orcutt [14], which unfortunately has not been published. Other references are [1], [9], [4]. First order systems have been studied extensively in [8]. Canonical systems are discussed in great detail in [5].

1.1. Regularity of the maximal relation

We consider again the system (1.1), (1.2).

Definition 1.5. We denote by S the closure in $L^2_{\mathscr{H}}(I) \times L^2_{\mathscr{H}}(I)$ of $S_{\min}$ and by $S_{\max} := S^* = \{\{f, g\} \in L^2_{\mathscr{H}}(I) \times L^2_{\mathscr{H}}(I) \mid \langle f, v \rangle = \langle g, u \rangle \text{ for all } \{u, v\} \in S\}$ the adjoint of S. Moreover, let

$$\mathscr{S}_{\max} := \{\{f, g\} \mid f, g \in \mathscr{L}^2_{\mathscr{H}}(I), f \in \mathrm{AC}(I, \mathbb{C}^n), Jf' + Bf = \mathscr{H}g\}.$$

The notation $\mathscr{S}_{\max}$ is deliberately chosen: if S is the graph of a symmetric first order operator as in (1.4) then it is well–known that each pair $\{\widetilde{f}, \widetilde{g}\}$ has representatives $\{f, g\} \in \mathscr{S}_{\max}$. It is exaggerating but true that this follows from elliptic regularity. For the system (1.1) the same statement holds true, although it is less obvious:

Theorem 1.6 (Regularity Theorem). *Let $\{\widetilde{f}, \widetilde{g}\} \in S_{\max}$. Then for each representative $g \in \widetilde{g}$ there exists $f \in \widetilde{f}$ such that $\{f, g\} \in \mathscr{S}_{\max}$.*

For definite systems this has been proved by Orcutt [14, Thm. II.2.6 and Thm. IV.2.5]. Another proof for (not necessarily definite) 2×2 canonical systems was given by I.S. Kac [7] in the deposited but unpublished elaboration of [6]. The proof of a more detailed version of Theorem 1.6 will be published in [10, Sec. 2].

We present an application of the regularity theorem: Let

$$\mathscr{E}_\lambda(S) := \{f \in \mathscr{L}^2_{\mathscr{H}}(I) \cap AC(I, \mathbb{C}^n) \mid Jf' + Bf = \lambda \mathscr{H} f\}, \qquad (1.12)$$

and denote by $\mathscr{N}_\pm(S) := \dim \mathscr{E}_{\pm i}(S)$ the *formal* deficiency indices of the system (1.1). Furthermore, for a symmetric linear relation A in the Hilbert space $\mathfrak{H}$ we denote by

$$E_\lambda(A) := \{f \in \mathfrak{H} \mid \{f, \lambda f\} \in A^*\}, \qquad \lambda \in \mathbb{C}, \qquad (1.13)$$

the defect subspace and by $N_\pm(A) := \dim E_{\pm i}(A)$ the deficiency indices of A. It is well–known that

$$\dim E_{\pm\lambda}(A) = N_\pm(A), \qquad \lambda \in \mathbb{C}_+ := \{z \in \mathbb{Z} \mid \mathrm{Im}\, z > 0\}. \qquad (1.14)$$

Namely, the relation $A^* - \lambda$ is semi–Fredholm for $\lambda \in \mathbb{C} \setminus \mathbb{R}$. Thus $\dim E_\lambda(A)$ is locally constant on $\mathbb{C} \setminus \mathbb{R}$ and therefore $\dim E_{\pm\lambda}(A) = \dim E_{\pm i}(A)$ for $\lambda \in \mathbb{C}_+$.

The same statement for the dimensions of the formal defect subspaces $\mathscr{E}_\lambda(S)$ is true but less trivial. The only proof we know of is due to Kogan and Rofe–Beketov [8, Sec. 2]. It uses methods from complex analysis and is rather technical. Using Theorem 1.6 we can give a painless proof of this fact:

Theorem 1.7 ([8, Theorem 2.1], [10, Sec. 2]). *Let S be a general symmetric system (1.1), (1.2) on an interval $I \subset \mathbb{R}$. If the system is definite or if the interval is half–closed, i.e. $I = [0, a)$, then*

$$\dim \mathscr{E}_{\pm\lambda}(S) = \dim \mathscr{E}_{\pm i}(S) =: \mathscr{N}_\pm(S), \quad \text{for} \quad \lambda \in \mathbb{C}_+.$$

Proof. 1. We assume first that the system S is definite. Then the quotient map $\mathscr{E}_\lambda(S) \to E_\lambda(S), f \mapsto \widetilde{f}$ is bijective.

Indeed, the injectivity follows immediately from the definition of definiteness. To prove surjectivity, consider $\widetilde{f} \in E_\lambda(S)$. This means $\{\widetilde{f}, \lambda\widetilde{f}\} \in S_{\max}$ and in view of Theorem 1.6 there exists $f \in \widetilde{f}, f \in \mathrm{AC}(I, \mathbb{C}^n) \cap \mathscr{L}^2_{\mathscr{H}}(I)$ such that $Jf' + Bf = \lambda\mathscr{H}f$. Thus $f \in E_\lambda(S)$. This proves surjectivity.

Now we have $\dim \mathscr{E}_\lambda(S) = \dim E_\lambda(S)$ and in view of (1.14) we reach the conclusion.

2. If S is not definite but $I = [0, a)$ we replace $\mathscr{H}$ by $\widetilde{\mathscr{H}} = \mathscr{H} + \chi I_n$, where χ is the characteristic function of an interval $[0, \varepsilon) \subset I$. The system $\widetilde{S} = S(J, B, \widetilde{\mathscr{H}})$ is definite on I and 1. applies. To complete the proof it remains to note that we obtain a linear isomorphism, Φ, from $\mathscr{E}_\lambda(S)$ onto $\mathscr{E}_\lambda(\widetilde{S})$ as follows: for $f \in \mathscr{E}_\lambda(S)$ let Φf be the solution of the differential equation $Jy' + By = \lambda\widetilde{\mathscr{H}}y$ with $\Phi f \restriction [\varepsilon, a) = f \restriction [\varepsilon, a)$. $\square$

1.2. Essential self–adjointness

In this section we study the system (1.1) on the real line and discuss criteria for essential self–adjointness. As a motivation, let $\{f, h\}$ be in the "square" of $\mathscr{S}_{\min}$, that is there is a $g \in \mathscr{L}^2_{\mathscr{H}}(I)$ such that $\{f, g\} \in \mathscr{S}_{\min}$ and $\{g, h\} \in \mathscr{S}_{\min}$. This is equivalent to the equation

$$\begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix}' + \begin{pmatrix} 0 & B \\ B & -\mathscr{H} \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} \mathscr{H} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} h \\ 0 \end{pmatrix}, \tag{1.15}$$

with $f, g \in \mathrm{AC}_{\mathrm{comp}}(I, \mathbb{C}^n), h \in \mathscr{L}^2_{\mathscr{H}, \mathrm{comp}}(I)$. A second example is the system discussed in Example 1.2. These examples lead us to consider a first order system

$$\widetilde{J}f' + \widetilde{B}f = \widetilde{\mathscr{H}}g, \tag{1.16}$$

where

$$\widetilde{J} = \begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix}, \quad \widetilde{B} = \begin{pmatrix} V & B \\ B & -A \end{pmatrix}, \quad \widetilde{\mathscr{H}} = \begin{pmatrix} \mathscr{H} & 0 \\ 0 & 0 \end{pmatrix}. \tag{1.17}$$

A is assumed to be nonnegative. V may be viewed as a "potential" added to $\mathscr{S}^2_{\min}$. It is clear that $L^2_{\widetilde{\mathscr{H}}}(I)$ is canonically isomorphic to $L^2_{\mathscr{H}}(I)$. We put $\widetilde{\mathscr{S}_{\min}} = \mathscr{S}(\widetilde{J}, \widetilde{B}, \widetilde{\mathscr{H}})$. For simplicity we will consider the interval $\mathbb{R}$ only. For a function $f \in \mathscr{L}^2_{\widetilde{\mathscr{H}}}(\mathbb{R})$ we denote by f_1, f_2 the first resp. last n components.

We will use several times that if $\mathscr{H}(x)$ and $A(x)$ are invertible then we can estimate, for $\xi, \eta \in \mathbb{C}^n$,

$$\begin{aligned} \left| \xi^* J\eta \right| &= \|A(x)^{1/2}\xi\| \|A(x)^{-1/2}J(x)\mathscr{H}(x)^{-1/2}\mathscr{H}(x)^{1/2}\eta\| \\ &\leq \|A(x)^{-1/2}J(x)\mathscr{H}(x)^{-1/2}\| \|A(x)^{1/2}\xi\| \|\mathscr{H}(x)^{1/2}\eta\|. \end{aligned} \tag{1.18}$$

Thus we put

$$c(x) := \begin{cases} \|A(x)^{-1/2}J(x)\mathscr{H}(x)^{-1/2}\|, & \det(A(x)\mathscr{H}(x)) \neq 0, \\ \infty, & \text{otherwise.} \end{cases} \tag{1.19}$$

The self–adjointness criterion we are going to present will depend also on V. We assume that there exists an absolute continuous function $q \geq 1$ on $\mathbb{R}$ such that

$$V \geq -q\mathscr{H}. \tag{1.20}$$

Lemma 1.8. *Let $f \in L^1_{\mathrm{loc}}(\mathbb{R})$, $f(x) \geq 0$, be a non–negative locally integrable function. Assume in addition that*

$$\pm \int_0^{\pm\infty} f(x)dx = +\infty. \tag{1.21}$$

Then there is a sequence of functions $\chi_n \in \mathrm{AC}_{\mathrm{comp}}(\mathbb{R})$ satisfying

$$0 \leq \chi_n \leq 1, \quad |\chi'_n| \leq \frac{1}{n}f(x), \quad \lim_{n\to\infty}\chi_n(x) = 1, \quad x \in \mathbb{R}. \tag{1.22}$$

Proof. Let $\chi \in C_0^\infty(\mathbb{R})$ with $0 \leq \chi \leq 1$, $\chi(x) = 1$ in a neighborhood of 0 and $|\chi'| \leq 1$. Then

$$\chi_n(x) := \chi\Big(\frac{1}{n}\int_0^x f(s)ds\Big) \tag{1.23}$$

does the job. $\square$

Lemma 1.9 ([16, Lemma 3.1], cf. Proposition 2.8 below). *Assume that*

$$\pm \int_0^{\pm\infty} \frac{1}{c(x)}dx = \infty,$$

and that $|\frac{d}{dx}q^{-1/2}(x)| \leq C/c(x)$. Let $\{f, g\} \in \widetilde{\mathscr{S}}_{\max}$. Then $q^{-1/2}f_2 \in \mathscr{L}^2_A(\mathbb{R})$ and

$$\|q^{-1/2}f_2\|_A \leq 2\Big((1 + 2C^2)\|f\|_{\widetilde{\mathscr{H}}}^2 + \|f\|_{\widetilde{\mathscr{H}}}\|g\|_{\widetilde{\mathscr{H}}}\Big).$$

Proof. By Lemma 1.8 there are absolute continuous functions χ_n with $0 \leq \chi_n \leq 1$, $\lim_{n\to\infty}\chi_n(x) = 1$, and

$$|\chi'_n(x)| \leq \frac{1}{nc(x)}. \tag{1.24}$$

Put $\psi_n := \chi_n q^{-1/2}$. We have

$$|\psi'_n(x)| \leq \Big(\frac{1}{n} + C\Big)\frac{1}{c(x)} =: C_n\frac{1}{c(x)}. \tag{1.25}$$

Then

$$\begin{aligned}
\|\psi_n f_2\|_A^2 &= \int_{\mathbb{R}} \psi_n^2(x)f_2^*(x)(Jf_1' + Bf_1)(x)dx \\
&= \int_{\mathbb{R}} \psi_n^2(J(x)f_2'(x) + B(x)f_2(x))^*f_1(x) - 2\int_{\mathbb{R}} \psi_n(x)\psi'_n(x)f_2(x)^*J(x)f_1(x)dx \\
&= \int_{\mathbb{R}} \psi_n(x)^2 g_1(x)^*\mathscr{H}(x)f_1(x)dx - \int_{\mathbb{R}} \psi_n(x)^2 f_1(x)^*V(x)f_1(x)dx \\
&\quad - 2\int_{\mathbb{R}} \psi_n(x)\psi'_n(x)f_2(x)^*J(x)f_1(x)dx.
\end{aligned} \tag{1.26}$$

Note that in view of (1.25) the matrices $A(x)$ and $\mathscr{H}(x)$ are invertible if $\psi_n'(x) \neq 0$. Combining (1.18), (1.20), (1.25), (1.26) and the well–known estimate $2|ab| \leq a^2 + b^2$ we obtain

$$
\begin{aligned}
\|\psi_n f_2\|_A^2 &\leq \left|\langle \psi_n^2 f, g\rangle_{\widetilde{\mathscr{H}}}\right| + \|\psi_n q^{1/2} f_1\|_{\mathscr{H}}^2 + 2C_n \|\psi_n f_2\|_A \|f\|_{\mathscr{H}} \\
&\leq \|f\|_{\widetilde{\mathscr{H}}}\|g\|_{\widetilde{\mathscr{H}}} + (1 + 2C_n^2)\|f\|_{\widetilde{\mathscr{H}}}^2 + \frac{1}{2}\|\psi_n f_2\|_A^2,
\end{aligned}
\tag{1.27}
$$

or

$$
\|\psi_n f_2\|_A^2 \leq 2\big((1 + 2C_n^2)\|f\|_{\widetilde{\mathscr{H}}}^2 + \|f\|_{\widetilde{\mathscr{H}}}\|g\|_{\widetilde{\mathscr{H}}}\big).
\tag{1.28}
$$

Letting $n \to \infty$ we reach the conclusion. $\qquad\square$

Theorem 1.10 ([16, Theorem 1.1], cf. Theorem 2.3 below). *On the interval* $\mathbb{R}$ *let* $\widetilde{J}, \widetilde{B}, \widetilde{\mathscr{H}}$ *be as in* (1.17) *with* $A \geq 0$. *Let* $q \geq 1$ *be absolute continuous and* $V \geq -q\mathscr{H}$. *Moreover, assume that*

(1) $\left|\frac{d}{dx}q^{-1/2}(x)\right| \leq \frac{C}{c(x)}$.

(2) $\pm \displaystyle\int_0^{\pm\infty} \frac{1}{c(x)q^{1/2}(x)}dx = \infty$.

Then $\widetilde{S} = S(\widetilde{J}, \widetilde{B}, \widetilde{\mathscr{H}})$ *is essentially self–adjoint.*

Proof. By Lemma 1.8 there are absolute continuous functions $\chi_n \in \mathrm{AC}_{\mathrm{comp}}(\mathbb{R})$, $0 \leq \chi_n \leq 1$, $\lim\limits_{n\to\infty} \chi_n(x) = 1$, and

$$
|\chi_n'(x)| \leq \frac{1}{nc(x)q^{1/2}(x)}.
\tag{1.29}
$$

Note that, again, $\chi_n'(x) \neq 0$ implies that $A(x)$ and $\mathscr{H}(x)$ are invertible. In view of the regularity Theorem 1.6 it suffices to show for $\{f, g\}, \{u, v\} \in \widetilde{\mathscr{S}}_{\max}$ that

$$
\langle f, v\rangle = \langle g, u\rangle.
\tag{1.30}
$$

By dominated convergence we have

$$
\lim_{n\to\infty} \big(\langle\chi_n f, v\rangle - \langle\chi_n g, u\rangle\big) = \langle f, v\rangle - \langle g, u\rangle.
\tag{1.31}
$$

Integration by parts shows that

$$
\begin{aligned}
\big(\langle\chi_n f, v\rangle - \langle\chi_n g, u\rangle\big) &= -\int_{\mathbb{R}} \chi_n'(x) f(x)^* \widetilde{J}(x) u(x)dx \\
&= -\int_{\mathbb{R}} \chi_n'(x)\big(f_1(x)^* J(x) u_2(x) + f_2(x)^* J(x) u_1(x)\big)dx.
\end{aligned}
\tag{1.32}
$$

Using (1.18) and Lemma 1.9 this can be estimated by

$$
\big|\langle\chi_n f, v\rangle - \langle\chi_n g, u\rangle\big| \leq \frac{1}{n}\big(\|f_1\|_{\mathscr{H}}\|q^{-1/2} u_2\|_A + \|q^{-1/2} f_2\|_A \|u_1\|_{\mathscr{H}}\big),
\tag{1.33}
$$

and we reach the conclusion. $\qquad\square$

Remark 1.11. We emphasize that Lemma 1.9, Theorem 1.10 and their proofs are adapted from a method due to M. Shubin [16] who proved essential self–adjointness for certain Schrödinger type operators on complete manifolds. A generalization of Shubin's method is presented below in the second part of this paper.

We single out some special cases of the previous theorem.

Corollary 1.12. *Consider the system $S_{\min} = S(J, B, \mathscr{H})$ as in (1.1) on $I = \mathbb{R}$. Put*

$$c(x) := \begin{cases} \|\mathscr{H}(x)^{-1/2} J(x) \mathscr{H}(x)^{-1/2}\|, & \det(\mathscr{H}(x)) \neq 0, \\ \infty, & \text{otherwise.} \end{cases} \tag{1.34}$$

Assume

$$\pm \int_0^{\pm\infty} \frac{1}{c(x)} dx = +\infty. \tag{1.35}$$

Then $S_{\min}$ and $S_{\min}^2$ are essentially self–adjoint, i.e. $\overline{S_{\min}} = S_{\max}$ and $\overline{S_{\min}^2} = (S^2)_{\max}$.

This corollary generalizes a result of Sakhnovich [15].

Proof. The essential self–adjointness of $S_{\min}^2$ follows, in view of (1.15), from Theorem 1.10 with $V = 0, q = 1$ and $A = \mathscr{H}$.

It is easy to see that, as in the case of a symmetric operator, the essential self–adjointness of the square of a s.l.r. in a Hilbert space implies the essential self–adjointness of the s.l.r. itself. However, the essential self–adjointness of $S_{\min}$ can easily be seen directly:

According to Lemma 1.8 let $\chi_n \in \mathrm{AC}_{\mathrm{comp}}(\mathbb{R})$ with $0 \leq \chi_n \leq 1$, $\lim\limits_{n\to\infty} \chi_n(x) = 1$, and

$$|\chi_n'(x)| \leq \frac{1}{nc(x)}. \tag{1.36}$$

For $\{\widetilde{f}, \widetilde{g}\} \in S_{\max}$ we choose, according to Theorem 1.6, representatives $\{f, g\} \in \mathscr{S}_{\max}$ and put $f_n := \chi_n f$. Since χ_n' vanishes if $\mathscr{H}(x)$ is not invertible the function $\chi_n' \mathscr{H}(x)^{-1} J f$ is well–defined. Moreover

$$\begin{aligned} \|\chi_n' \mathscr{H}^{-1} J f\|_{L^2_{\mathscr{H}}(\mathbb{R})}^2 &\leq \int_{\mathbb{R}} |\chi_n'(x)|^2 f(x)^* J(x)^* \mathscr{H}(x)^{-1} J(x) f(x) dx \\ &\leq \sup_{x\in\mathbb{R}} (\chi_n'(x) c(x))^2 \|f\|_{L^2_{\mathscr{H}}(\mathbb{R})}^2 \\ &\leq \frac{1}{n^2} \|f\|_{L^2_{\mathscr{H}}(\mathbb{R})}^2, \end{aligned}$$

hence $\chi_n' \mathscr{H}(x)^{-1} J f$ lies in $\mathscr{L}^2_{\mathscr{H}}(\mathbb{R})$ and it converges to 0 in $\mathscr{L}^2_{\mathscr{H}}(\mathbb{R})$. Finally, we calculate

$$\begin{aligned} J f_n' + B f_n &= \chi_n (J f' + B f) + \chi_n' J f \\ &= \mathscr{H}(\chi_n g + \chi_n' \mathscr{H}^{-1} J f) \\ &=: \mathscr{H} g_n. \end{aligned}$$

Thus $\{f_n, g_n\} \in \mathscr{S}_{\min}$ and $\lim\limits_{n\to\infty} \{\widetilde{f}_n, \widetilde{g}_n\} = \{\widetilde{f}, \widetilde{g}\}$ and the claim is proved. $\qquad\square$

Corollary 1.13. *Let $S_{\min}$ be the symmetric linear relation in $L^2_{\mathscr{H}}(\mathbb{R})$ induced by the Sturm–Liouville type equation*

$$-\frac{d}{dx}\big(A(x)^{-1}\frac{d}{dx}u(x)\big) + V(x)u(x) = \mathscr{H}(x)v(x). \qquad (1.37)$$

That is, $\{\widetilde{u}, \widetilde{v}\} \in S_{\min}$ if and only if there exist $u \in \widetilde{u}, v \in \widetilde{v}$ such that $u, A^{-1}\frac{d}{dx}u \in \mathrm{AC}_{\mathrm{comp}}(\mathbb{R}, \mathbb{C}^n), v \in \mathscr{L}^2_{\mathscr{H},\mathrm{comp}}(\mathbb{R})$ and (1.37) holds. Here, we assume that $A, V, \mathscr{H} \in L^1_{\mathrm{loc}}(\mathbb{R}, \mathrm{M}(n, \mathbb{C})), A(x)$ is positive definite for all $x \in \mathbb{R}$, and that there exists an absolute continuous function $q \geq 1$ such that $V \geq -q\mathscr{H}$. Let $c(x)$ be defined by (1.19). Moreover, assume that

(1) $\left|\frac{d}{dx}q^{-1/2}(x)\right| \leq \frac{C}{c(x)}.$

(2) $\pm \int_0^{\pm\infty} \frac{1}{c(x)q^{1/2}(x)}dx = \infty.$

Then $S_{\min}$ is essentially self–adjoint.

Proof. This follows immediately from Theorem 1.10, (1.5), and (1.6). □

Proposition 1.14. *Under the assumptions of Theorem 1.10 the system $\widetilde{S} = S(\widetilde{J}, \widetilde{B}, \widetilde{\mathscr{H}})$ is definite.*

Proof. Consider $f \in \mathscr{L}^2_{\mathscr{H}}(\mathbb{R}) \cap \mathrm{AC}(\mathbb{R}, \mathbb{C}^{2n})$ satisfying

$$\widetilde{J}f' + \widetilde{B}f = 0, \qquad \int_{\mathbb{R}} f^*\widetilde{\mathscr{H}}f = 0. \qquad (1.38)$$

We have to show that $f = 0$. (1.38) translates into

$$Jf'_1 + Bf_1 - Af_2 = 0, \qquad (1.39)$$
$$Jf'_2 + Bf_2 + Vf_1 = 0, \qquad (1.40)$$
$$\int_{\mathbb{R}} f_1^*\mathscr{H}f_1 = 0. \qquad (1.41)$$

Note that condition (2) in Theorem 1.10 implies that $A(x)$ and $\mathscr{H}(x)$ are invertible on a set of positive Lebesgue measure. Consequently, the systems $\mathscr{S}(J, B, A), \mathscr{S}(J, B, \mathscr{H})$ are definite.

From Lemma 1.9 and (1.41) we infer $\|f_2\|_A = 0$. Hence $Af_2 = 0$ a.e. Since $\mathscr{S}(J, B, \mathscr{H})$ is definite we infer from (1.39) and (1.41) that $f_1 = 0$. In view of (1.40) and $Af_2 = 0$ a.e. we may apply the definiteness of $\mathscr{S}(J, B, A)$ to conclude that $f_2 = 0$. □

2. First and second order operators on complete Riemannian manifolds

Let M be a connected complete Riemannian manifold. Furthermore, let E be a hermitian vector bundle over M. We denote by $L^2(E)$ the Hilbert space of square integrable sections of E with respect to the scalar product

$$(u, v) = \int_M \langle u(p), v(p)\rangle_{E_p}d\,\mathrm{vol}(p). \qquad (2.1)$$

Note that (2.1) is well–defined also if u is only locally square integrable and v has compact support, or vice versa. $L^2_{\text{loc}}(E), L^2_{\text{comp}}(E)$ denote the space of sections of E which are locally square integrable resp. square integrable with compact support. Sometimes it will be convenient to consider distributional sections of E. We denote by $C^{-\infty}(E)$ the (anti)dual space of $C^\infty_0(E)$ with respect to the anti-dual pairing (2.1).

Next we consider a second hermitian vector bundle, F, and a first order differential operator

$$D : C^\infty_0(E) \longrightarrow C^\infty_0(F). \tag{2.2}$$

Note that we do *not* assume D to be elliptic. We denote by D^t the formal adjoint of D, i.e. for compactly supported sections $u \in C^\infty_0(E), v \in C^\infty_0(F)$ one has

$$(Du, v) = (v, D^t u). \tag{2.3}$$

Thus D, D^t extend to maps on distributional sections of E, F and we will write $Du, D^t v$ also if u, v are distributional sections of E, F, resp. (mostly u, v will at least be locally square integrable).

Furthermore, let $\hat{D}$ be the principal symbol of D. Then for $u \in C^{-\infty}(E)$ and $\phi \in C^\infty(M)$ one has

$$D(\phi u) = \hat{D}(d\phi)u + \phi Du. \tag{2.4}$$

Remark 2.1. (2.4) holds whenever all ingredients make sense, in particular if $u \in L^2_{\text{loc}}(E), Du \in L^2_{\text{loc}}(E)$ and ϕ is a locally Lipschitz function.

Note that the defining relation (2.4) for the principal symbol implies that

$$\hat{D}^t(\xi) = -(\hat{D}(\xi))^*, \qquad \xi \in T^*_p M. \tag{2.5}$$

We consider D as an unbounded operator from $L^2(E)$ into $L^2(F)$. We denote by D_{min} the closure of D and by $D_{\text{max}} = (D^t)^* = ((D^t)_{\text{min}})^*$. In general one has $D_{\text{min}} \subsetneqq D_{\text{max}}$. Actually, $D_{\text{min}} = D_{\text{max}}$ is equivalent to the essential self–adjointness of the operator

$$\begin{pmatrix} 0 & D^t \\ D & 0 \end{pmatrix}. \tag{2.6}$$

Next we consider the Schrödinger operator

$$H := D^t D + V, \tag{2.7}$$

where $V \in L^\infty_{\text{loc}}(\text{End}(E))$ is a locally bounded self–adjoint (i.e. for each $p \in M$ the endomorphism $V(p) : E_p \to E_p$ is self–adjoint) potential.

H is a symmetric operator in $L^2(E)$ with domain $C^\infty_0(E)$. As for D we denote by H_{min} the closure of H and $H_{\text{max}} = H^* = H^*_{\text{min}}$.

Definition 2.2. Let M be a complete Riemannian manifold and let $0 < \varrho \leq 1$ be a locally Lipschitz function. We write

$$\int^{\infty} \varrho \, ds = \infty, \tag{2.8}$$

if $\int_0^{\infty} \varrho(\gamma(t))|\gamma'(t)| \, dt = \infty$ for any parametrized curve $\gamma : [0, \infty) \to M$ satisfying $\lim\limits_{t \to \infty} \gamma(t) = \infty$. The latter limit is taken in the one–point compactification of M, i.e. $\gamma(t)$ eventually leaves any compact subset $K \subset M$.

Finally, put $c(x) := \max(1, |\hat{D}(x)|)$. $c(x)$ is an upper estimate for the propagation speed of D. Now we can state the main result of this section:

Theorem 2.3. *Let $q \geq 1$ be a locally Lipschitz function such that $V \geq -q$. Moreover, assume that*

(1) $c|d(q^{-1/2})| \leq C$,

(2) $\displaystyle\int^{\infty} \frac{ds}{c\sqrt{q}} = \infty$,

(3) *if $u \in \mathscr{D}(H_{\max})$ then $Du \in L^2_{\mathrm{loc}}(F)$.*

Then the operator H is essentially self–adjoint on $C_0^{\infty}(E)$.

We comment on the assumptions and discuss some special cases:

Remark 2.4. 1. We emphasize, that the method presented here is essentially the one of Shubin [16, 17], modulo necessary changes due to the more general class of operators under consideration. We found it however worthwhile to show that in principle all operators of the form $D^t D + V$ can be dealt with in a unified way, going much beyond the class of Laplace type operators.

Note also the similarity between Theorem 2.3 and Theorem 1.10. Theorem 1.10, in fact, was inspired by Theorem 2.3.

2. The assumption (3) is automatically fulfilled if $D^t D$ is elliptic, or, more generally, if $D^t D$ is elliptic on a "sufficiently large" subset (see Proposition 2.9 below). We tried hard to prove the following conjecture:

Conjecture 2.5. *Let $T : C_0^{\infty}(E) \to C_0^{\infty}(E)$ be a first order differential operator on a Riemannian manifold and assume that T^2 is essentially self–adjoint. Let $u \in L^2_{\mathrm{loc}}(E), T^2 u \in L^2_{\mathrm{loc}}(E)$. Then $Tu \in L^2_{\mathrm{loc}}(E)$.*

Let us first comment on why this conjecture is conceivable. If T^2 is essentially self–adjoint then T is also essentially self–adjoint and $\overline{T^2} = \overline{T}^2$. Hence, if $u \in L^2(E), T^2 u \in L^2(E)$ then

$$\begin{aligned}
u \in \mathscr{D}(\overline{T^2}) &= \left\{ v \in L^2(E) \mid T^2 v \in L^2(E) \right\} \\
&= \mathscr{D}(\overline{T}^2) = \left\{ v \in L^2(E) \mid Tv, T^2 v \in L^2(E) \right\}.
\end{aligned} \tag{2.9}$$

Consequently, $Tu \in L^2(E)$. So, if we remove the "loc" subscripts then the statement of the conjecture holds. Now, since T is a differential operator, it is hard to believe that the validity of the conclusion depends on global properties of u. If one believes that the statement is a purely local one then it should be true even without the essential self–adjointness assumption on T^2, since every symmetric first order differential operator T can be altered outside a compact set in such a way that all powers become essentially self–adjoint (cf. the proof of Proposition 2.9 below). Maybe it is possible to prove (or disprove) the conjecture by micro-local methods. This we did not try too hard.

In Proposition 2.11 below it is proved that the conjecture in conjunction with condition (2) implies condition (3).

3. Let $V = 0$ and $q = 1$. Then we obtain the essential self–adjointness of $D^t D$ if $\int^{\infty} \frac{1}{c} = \infty$. This is exactly Chernoff's condition [3, Thm. 1.3]. Note that if $D^t D$ is elliptic then our method of proof is independent of Chernoff's paper. If $D^t D$ is non–elliptic we have to use Chernoff's results in the proof of Proposition 2.9 (and also in the proof of Proposition 2.11). It is an interesting question whether this Proposition could be proved by more elementary means.

If D is a generalized Dirac operator then D is elliptic and $c = 1$. Hence we obtain the essential self–adjointness of D^2 (and thus of D, too). In this case, however, our proof is very similar to the one of Wolf [18].

4. If $c = 1$ then Theorem 2.3 contains the main results in [11, 12, 13, 16, 17, 2] as special cases. Note that loc. cit. mostly deal with cases where $D^t D$ is a generalized Laplace operator. In this case, the integrand of $(Hu, v) - (u, Hv)$ can be expressed explicitly in terms of a divergence. These explicit divergence formulas are used in an essential way. We emphasize that our method works without such explicit formulas. The substitute for them is a more elaborate use of the calculus of unbounded operators in Hilbert space.

In particular, we wanted to include all Dirac type operators. For those, of course, the explicit divergence formulas could be worked out, although it would be somewhat tedious.

The magnetic Schrödinger operator considered in [17] is a priori not covered by Theorem 2.3 if the magnetic potential is not smooth. However, if $D^t D$ is elliptic, our proof can easily be adapted to the case that the 0th order part of D is only Lipschitz. For the sake of a simpler presentation, however, we will confine ourselves to the case of an operator D with smooth coefficients.

2.1. Some Preparations

(2.3) holds in greater generality:

Lemma 2.6. *Let $u \in \mathscr{D}(D_{\max}) \cap L^2_{\mathrm{comp}}(E)$ and $v \in L^2_{\mathrm{loc}}(F)$ such that $D^t v \in L^2_{\mathrm{loc}}(F)$. Then $u \in \mathscr{D}(D_{\min})$ and*

$$(Du, v) = (u, D^t v). \tag{2.10}$$

Proof. $u \in \mathscr{D}(D_{\min})$ follows easily by means of a Friedrich's mollifier constructed in a neighborhood of the compact support of u.

Next choose a cut–off function $\phi \in C_0^\infty(M)$ with $\phi \equiv 1$ in a neighborhood of $\operatorname{supp} u$. Then, $\phi v \in \mathscr{D}(D_{\max}^t)$ and hence

$$
\begin{aligned}
(Du, v) &= (\phi Du, v) \\
&= (D_{\min} u, \phi v) \\
&= (u, D_{\max}^t \phi v) \\
&= (u, -\hat{D}(d\phi)^* v + \phi D^t v) \\
&= (u, D^t v),
\end{aligned}
\tag{2.11}
$$

since $\operatorname{supp} d\phi \cap \operatorname{supp} u = \emptyset$. $\square$

Lemma 2.7 (cf. Lemma 1.8). *Let $\varrho \geq 1$ be a locally Lipschitz function on M with $\int^\infty \frac{ds}{\varrho} = \infty$. Then there is a sequence of Lipschitz functions (ϕ_n) with compact support satisfying*

$$
0 \leq \phi_n \leq 1, \quad |d\phi_n| \leq \frac{1}{\varrho n}, \quad \lim_{n\to\infty} \phi_n(x) = 1, \quad x \in M.
\tag{2.12}
$$

Proof. Denote by d_ϱ the distance function with respect to the metric $g_\varrho = \varrho^{-2} g$. Then fix $x_0 \in M$ and put $P(x) = d_\varrho(x, x_0)$. As in [16] one concludes $\lim_{x\to\infty} P(x) = \infty$ and $|dP| \leq \varrho^{-1}$. Now choose a cut–off function $\chi \in C_0^\infty(\mathbb{R})$ with $0 \leq \chi \leq 1$, $\chi = 1$ near 0, and $|\chi'| \leq 1$. Then put

$$
\phi_n(x) = \chi\left(\frac{P(x)}{n}\right).
\tag{2.13}
$$

ϕ_n obviously has the desired properties. $\square$

Proposition 2.8. *Assume that $\int^\infty \frac{ds}{c} = \infty$ and $c|d(q^{-1/2})| \leq C$. Let $u \in \mathscr{D}(H_{\max})$ and $Du \in L_{\mathrm{loc}}^2(F)$. Then we have $q^{-1/2} Du \in L^2(F)$ and*

$$
\|q^{-1/2} Du\| \leq 2\left((1 + 2C^2)\|u\|^2 + \|u\|\|Hu\|\right).
\tag{2.14}
$$

Proof. Let $0 \leq \psi \leq q^{-1/2}$ be a locally Lipschitz function with compact support and put $\widetilde{C} = \sup_{p \in M} c(p)|d\psi(p)|$.

Using Lemma 2.6 we find

$$
\begin{aligned}
(\psi Du, \psi Du) &= (D^t \psi^2 Du, u) \\
&= 2(\psi \hat{D}^t(d\psi) Du, u) + (\psi^2 D^t Du, u) \\
&= 2(\psi \hat{D}^t(d\psi) Du, u) + (\psi Hu, u) - (V\psi u, \psi u) \\
&\leq 2\widetilde{C}\|u\|\|\psi Du\| + \|u\|\|Hu\| + \|\psi q^{1/2} u\|^2 \\
&\leq 2\widetilde{C}\|u\|\|\psi Du\| + \|u\|\|Hu\| + \|u\|^2.
\end{aligned}
\tag{2.15}
$$

Using $2|ab| \leq a^2 + b^2$ the latter can be estimated

$$
\|\psi Du\|^2 \leq (1 + 2\widetilde{C}^2)\|u\|^2 + \frac{1}{2}\|\psi Du\|^2 + \|u\|\|Hu\|,
\tag{2.16}
$$

and thus

$$\|\psi Du\|^2 \le 2\Big((1 + 2\widetilde{C}^2)\|u\|^2 + \|u\|\|Hu\|\Big). \tag{2.17}$$

We apply Lemma 2.7 with $\varrho = c$ and obtain a sequence (ϕ_n) of Lipschitz functions ϕ_n which satisfy (2.12) with $\varrho = c$. Putting $\psi_n = \phi_n q^{-1/2}$ we have $0 \le \psi_n \le q^{-1/2}$ and

$$c|d\psi_n| \le cq^{-1/2}|d\phi_n| + \phi_n c|d(q^{-1/2})|$$
$$\le \frac{1}{n} + C. \tag{2.18}$$

Since $\psi_n(p) \to q^{-1/2}(p)$ as $n \to \infty$ we reach the conclusion by invoking the dominated convergence theorem. $\qquad\square$

2.2. Proof of the Main Theorem 2.3

Let $u, v \in \mathscr{D}(H_{\max})$ and let $0 \le \phi$ be a Lipschitz function with compact support. Since $q \ge 1$ the condition (2) implies for any curve $\gamma : [0, \infty)$ as in Definition 2.2

$$\int_0^\infty \frac{1}{c(\gamma(t))}|\gamma'(t)|dt \ge \int_0^\infty \frac{1}{c(\gamma(t))\sqrt{q(t)}}|\gamma'(t)|dt = \infty, \tag{2.19}$$

hence we can apply Proposition 2.8 and find that $q^{-1/2}Du, q^{-1/2}Dv \in L^2(F)$. Moreover, since ϕ has compact support, we have $\hat{D}(d\phi)u \in L^2_{\mathrm{comp}}(F)$. Also, since V is locally bounded, $D^t Du, D^t Dv \in L^2_{\mathrm{loc}}(E)$. Finally, the latter implies in view of

$$D^t \phi Du = -\hat{D}(d\phi)^* Du + \phi D^t Du \in L^2(E). \tag{2.20}$$

Using Lemma 2.6 and Remark 2.1 we calculate

$$(\phi u, D^t Dv) = (D\phi u, Dv)$$
$$= (\hat{D}(d\phi)u, Dv) + (\phi Du, Dv), \tag{2.21}$$

and, similarly,

$$(D^t Du, \phi v) = (Du, \hat{D}(d\phi)v) + (\phi Du, Dv). \tag{2.22}$$

Taking differences we obtain

$$|(\phi u, Hv) - (Hu, \phi v)| \le |(\hat{D}(d\phi)u, Dv)| + |(Du, \hat{D}(d\phi)v)|$$
$$\le \sup_{p \in M}\Big(|q^{1/2}(p)|\hat{D}(d\phi)|\Big)\big(\|u\|\|q^{-1/2}Dv\| + \|q^{-1/2}Du\|\|v\|\big). \tag{2.23}$$

Finally we invoke Lemma 2.7 with $\varrho = cq^{1/2}$ and choose a sequence of Lipschitz functions ϕ_n with compact support satisfying $0 \le \phi_n \le 1$, $|d\phi_n| \le \frac{1}{nc\sqrt{q}}$, $\lim_{n\to\infty} \phi_n(p) = 1, p \in M$. Then by dominated convergence we have on the one hand

$$(\phi_n u, Hv) - (Hu, \phi_n v) \longrightarrow (u, Hv) - (Hu, v), \qquad n \to \infty, \tag{2.24}$$

and on the other hand

$$|(\phi_n u, Hv) - (Hu, \phi_n v)| \le \frac{1}{n}\big(\|u\|\|q^{-1/2}Dv\| + \|q^{-1/2}Du\|\|v\|\big). \tag{2.25}$$

This proves the claim.

2.3. On condition (3) and Conjecture 2.5

Proposition 2.9. *Assume that there are compact subsets $K_n \subset M$ such that*

(1) $K_n \subset K_{n+1}$,

(2) $\bigcup\limits_{n=1}^{\infty} K_n = M$,

(3) *there is an open neighborhood $U_n \supset K_n$ such that $D^t D$ is elliptic in $U_n \setminus K_n$.*

Let $u \in \mathscr{D}(H_{\max})$. Then $Du \in L^2_{\text{loc}}(F)$.

Proof. 1. We note first that if $D^t D$ is elliptic (everywhere) then this is an easy consequence of elliptic regularity. Namely, if $Hu = v \in L^2_{\text{loc}}(E)$ then $D^t Du = v - Vu \in L^2_{\text{loc}}(E)$ and hence by elliptic regularity this implies $u \in H^2_{\text{loc}}(E)$. I.e. u is locally of Sobolev class H^2 and hence in particular $Du \in L^2_{\text{loc}}(E)$.

2. If $D^t D$ is not elliptic everywhere then we have to invoke the hyperbolic equation method as presented e.g. by P. R. Chernoff [3]. As in 1. we have $D^t Du \in L^2_{\text{loc}}(E)$ and hence, by elliptic regularity, $u \restriction U_n \setminus K_n$ is locally of Sobolev class H^2, in particular $(Du) \restriction U_n \setminus K_n$ is locally square integrable.

We now show that $(Du) \restriction K_n$ is square integrable. Choose a large compact set $K \supset U_n$ and let $\widetilde{D}$ be a first order differential operator which coincides with D over K and which vanishes outside a large compact set L. Now consider the operator

$$T := \begin{pmatrix} 0 & \widetilde{D}^t \\ \widetilde{D} & 0 \end{pmatrix}. \tag{2.26}$$

T is a formally symmetric differential operator which vanishes outside a compact set. Hence, T has bounded propagation speed, in particular it satisfies Chernoff's condition $\int^{\infty} \frac{ds}{c} = \infty$. Thus by the hyperbolic equation method [3] all powers of T are essentially self–adjoint.

Next choose a cut–off function $\phi \in C_0^{\infty}(M)$ with $\phi \equiv 1$ in a neighborhood of K_n and $\text{supp}\,\phi \subset U_n$. Then the commutator $[D^t D, \phi] = [\widetilde{D}^t \widetilde{D}, \phi]$ is a first order differential operator which is supported in $U_n \setminus K_n$. In particular $[\widetilde{D}^t \widetilde{D}, \phi]u \in H^1_{\text{comp}}(E)$ and hence $\widetilde{D}^t \widetilde{D}(\phi u) = [\widetilde{D}^t \widetilde{D}, \phi]u + \phi \widetilde{D}^t \widetilde{D}u = [\widetilde{D}^t \widetilde{D}, \phi]u + \phi D^t Du \in L^2(E)$. Then

$$T^2 \begin{pmatrix} \phi u \\ 0 \end{pmatrix} = \begin{pmatrix} \widetilde{D}^t \widetilde{D} \phi u \\ 0 \end{pmatrix} \tag{2.27}$$

is square integrable. Since T^2 is essentially self–adjoint, this implies that

$$\begin{pmatrix} \phi u \\ 0 \end{pmatrix} \in \mathscr{D}(\overline{T^2}) = \mathscr{D}(\overline{T}^2) = \left\{ v \in L^2(E \oplus E) \mid Tv, T^2 v \in L^2(E \oplus E) \right\}, \tag{2.28}$$

hence

$$T \begin{pmatrix} \phi u \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ D(\phi u) \end{pmatrix} \tag{2.29}$$

is square integrable. This implies that $(Du) \restriction K_n$ is square integrable. $\qquad\square$

Remark 2.10. If D^tD is not elliptic in the shells $U_n \setminus K_n$ then in the proof of 2. we face the difficulty that there is no obvious way to construct enough cut–off functions ϕ such that $D^tD(\phi u) \in L^2(E)$. It would be enough to show the following: given $u \in L^2_{\text{loc}}(E), D^tDu \in L^2_{\text{loc}}(E)$ then there is a $v \in L^2_{\text{comp}}(E), D^tDv \in L^2_{\text{comp}}(E)$ such that $v \upharpoonright K_n = u$. v does not necessarily have to be of the form ϕu.

Proposition 2.11. *Assume that Conjecture* 2.5 *holds. Then condition* (2) *in Theorem* 2.3 *implies condition* (3).

Proof. Since $q \geq 1$ the condition (2) implies $\int^\infty \frac{ds}{c} = \infty$ (cf. (2.19)), hence the symmetric operator (2.26) satisfies Chernoff's condition [3, Thm. 1.3]. Thus all powers of T are essentially self–adjoint. Now, if $u \in \mathscr{D}(H_{\max})$ then $D^tDu \in L^2_{loc}(E)$ and hence

$$\widetilde{u} := \begin{pmatrix} u \\ 0 \end{pmatrix} \tag{2.30}$$

satisfies $\widetilde{u} \in L^2_{\text{loc}}(E \oplus E), T^2\widetilde{u} \in L^2_{\text{loc}}(E \oplus E)$. Consequently, Conjecture 2.5 implies

$$T\widetilde{u} = \begin{pmatrix} 0 \\ Du \end{pmatrix} \in L^2_{\text{loc}}(F \oplus F), \tag{2.31}$$

and thus $Du \in L^2_{\text{loc}}(F)$. □

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THE UNIVERSITY OF ARIZONA, DEPARTMENT OF MATHEMATICS, 617 N. SANTA RITA, TUCSON, AZ 85721–0089, USA
lesch@math.arizona.edu
www.math.arizona.edu/∼lesch